PULSED-FIELD IONOZATION ELECTRON SPECTROSCOPY OF LANTHANIDE (Lu, Gd) BENZENE COMPLEXES

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Over the last 25 years, organometallic chemistry of f elements has attracted considerable attentions of both experimentalists and theoreticians. We have recently succeeded in producing Ln-benzene (Ln = Lu, Gd) complexes in laser-vaporization supersonic molecular beams and in measuring their vibronic spectra using single-photon pulsed field ionization-zero electron kinetic energy (PFI-ZEKE) spectroscopy. We obtained for the first time the adiabatic ionization energy (AIE) and metal-benzene vibrational frequencies. The AIE of the Lu-benzene complex is 44461 (5) cm^{-1}, and the Lu-benzene stretching frequencies are 204 and 270 cm^{-1} in the neutral and ion, respectively. For the Gd-benzene complex, its AIE is 40830 (5) cm^{-1}, and the metal-ligand stretching frequencies of the neutral and ionic species are 256 and 298 cm^{-1}. We will discuss the electronic transitions involved in the PFI-ZEKE spectra of the two complexes by combining the experimental measurements with quantum chemical calculations and spectral simulations.